CHAPTER V

CONCLUSION

We have presented in this thesis the photoemission calculations by using a simple dielectric model as given by Bagchi and Kar[21]. We have calculated at first the variation of the electromagnetic field against the photon energy for planes located in the surface region. The solids for which the fields was calculated are the metals aluminium, silver, rhodium, molybdenum, palladium and the semiconductor silicon. In most cases we saw that instead of a monotonic behaviour, there was a lot of structure associated with the field variation, either as a function of energy or as a function of position.

We have next done a photoemission calculation with the photon field described as above and the initial and final state wavefunctions chosen to be free-electron wavefunctions in the presence of a surface. Since aluminium is a prototype free electron metal, numerical calculations were performed with the parameters appropriate for aluminium and the results compared with experimental data as well as previously calculated results. It was seen that qualitative agreement was obtained, even with this simple model.

As a first step towards including band structure effects, another model calculation was performed - this time considering

a Kronig - Penney model for the initial state wavefunction. As input for field calculation, the data for aluminium, tungsten and silicon were used, with the potential parameters kept the same. We could then see the influence of the optical parameters by comparing the results. As expected, the plasmon frequency has an important role in these calculations. It was seen that the photocurrent showed a peak at photon energy less than the plasmon energy and a minimum at the plasmon energy. Photocurrent calculations by using the same initial state and the final state wavefunctions was also done but with no surface region included. In this case the usual peak below the plasmon energy was not exhibited by the photocurrent data nor the minimum at the plasmon energy. This therefore led us to conclude that the inclusion of surface is important in photoemission calculations.

We have done photoemission calculations with simple models in this thesis. To include real band structure effects, we need a more realistic type of initial state wavefunction which in its true sense would be able to describe the actual configuration of the electronic states of the solids under investigation. However, we see that our calculations lead us to conclude that the spatial variation of electromagnetic field in the surface regions plays an important role during photoemission, which should be taken into account in more accurate photocurrent calculations.